A Method for Calculating Pressure Profiles in Vacuum Pipes

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Abstract

A technique for calculating the pressure profile of a very long and complicated vacuum chamber is presented. The technique uses the approximation of *finite differences* to cast the problem into a linear form that can readily be solved by matrix manipulations. The procedure is fast and numerically stable. A program is described that uses this procedure and has a simple, modular input structure. The program can also calculate pressure profiles for complicated beam pipe structures like those found in a B factory interaction region design.

INTRODUCTION.

Various methods have been developed to compute the pressure profile of vacuum chambers used in accelerators and storage rings [1-2]. However, these methods rely on formulas that are similar to beam transport formalisms and suffer from numerical instabilities when the vacuum chamber under study gets too long.

The pressure profile in a vacuum chamber where the gas pressure is low enough to ignore viscosity is governed by the following differential equation over regions in which the conductance is constant [3]:

$$c\frac{d^2P}{dz^2} - sP + q = 0 \qquad (1)$$

where

P = pressure [nTorr]

c = specific molecular conductance [m(l/s)]

s = specific linear pumping speed [(l/s)/m]

q = specific outgas rate [nTorr(l /s)/m].

The general solution of this differential equation (homogeneous + inhomogeneous) is:

$$P(z) = C_1 e^{\alpha z} + C_2 e^{-\alpha z} + \frac{q}{c} \qquad (2)$$

with $\alpha = \sqrt{\frac{s}{c}}$.

BEAM TRANSFER MATRIX FORMALISM.

The above general solution can be cast into a transfer matrix formalism. One then gets the following matrix equation for each vacuum chamber element of length L.

$$\begin{pmatrix} P(L) \\ \frac{dP}{dz}(L) \\ 1 \end{pmatrix} = \begin{pmatrix} \cosh(\alpha L) & \frac{1}{\alpha}\sinh(\alpha L) & -\frac{q}{c\alpha^2}(\cosh(\alpha L)-1) \\ \alpha\sinh(\alpha L) & \cosh(\alpha L) & -\frac{q}{c\alpha}\sinh(\alpha L) \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} P_0 \\ \frac{dP_0}{dz} \\ 1 \end{pmatrix}$$

or with $Q = -c\frac{dP}{dz}$ we have:

$$\begin{pmatrix} P(L) \\ Q(L) \\ 1 \end{pmatrix} = \begin{pmatrix} \cosh(\alpha L) & -\frac{1}{c\alpha}\sinh(\alpha L) & -\frac{q}{c\alpha^2}(\cosh(\alpha L)-1) \\ -c\alpha\sinh(\alpha L) & \cosh(\alpha L) & \frac{q}{\alpha}\sinh(\alpha L) \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} P_0 \\ Q_0 \\ 1 \end{pmatrix}$$

One can then multiply the matrices found for each element of a beam pipe together to get an overall transfer matrix. Then, given two of the four boundary conditions, one can solve for the other two boundary conditions. Once the boundary conditions are known at each end of the pipe, one can select one end of the pipe and use the matrices defined for each pipe element to calculate the pressure and flow at the ends of every pipe element. The difficulty of the above formalism is with the exponential terms in the hyperbolic sine and cosine functions. As the beam pipe under study gets longer, the exponent gets larger, producing large entries in the transfer matrix. The matrix can not be rescaled to get rid of these large numbers because the last row of the matrix always remains the same. In order to maintain calculational accuracy, computer precision has to be increased. Using "QUAD" precision (33 digits of accuracy on a VAX), one is able to calculate a pressure profile of beam pipes that are no more than about 30 meters long. The basic problem of this formalism is that the overall transfer matrix, as defined above, is a measure of the correlation between the boundary conditions at one end of a pipe with the other end. As the length of the pipe grows, this correlation becomes vanishingly small. Hence, the matrix gets closer and closer to being singular.

FINITE DIFFERENCE METHOD.

Another approach to the problem of calculating pressure profiles is to segment each element of the beam pipe into small, equal sections of z and recast the derivatives as finite differences. However, equation (1) is valid only in regions in which the conductance is constant. In order to account for changes in pipe conductance, we use a slightly more general formula [4]:

$$\frac{d}{dz}\left(c\frac{dP}{dz}\right) - sP + q = 0 \qquad (3)$$

This equation insures that the pressure P and the flow Q (= –c dP/dz) are continuous. One then gets the following finite difference for the double derivative in each small segment of the pipe:

$$\frac{d}{dz}\left(c_i \frac{dP_i}{dz}\right) = \frac{c_{i+1/2}\frac{dP_{i+1/2}}{dz} - c_{i-1/2}\frac{dP_{i-1/2}}{dz}}{\Delta z}$$

$$= \frac{c_{i+1/2}\frac{P_{i+1} - P_i}{\Delta z} - c_{i-1/2}\frac{P_i - P_{i-1}}{\Delta z}}{\Delta z}$$

$$= \frac{c_{i+1/2}P_{i+1} + c_{i-1/2}P_{i-1} - (c_{i+1/2}+c_{i-1/2})P_i}{\Delta z^2}$$

$$= \frac{(c_{i+1}+c_i)P_{i+1} + (c_i+c_{i-1})P_{i-1} - (c_{i+1}+c_{i-1}+2c_i)P_i}{2\Delta z^2} \quad . \qquad (4)$$

One then has a series of segments each with the following equation

$$\frac{(c_{i+1}+c_i)P_{i+1} + (c_i+c_{i-1})P_{i-1} - (c_{i+1}+c_{i-1}+2c_i)P_i}{2\Delta z^2} - s_i P_i + q_i = 0 \quad .$$

Combining terms we have

$$\frac{c_i + c_{i-1}}{2}P_{i-1} + \left(-\frac{c_{i+1} + c_{i-1} + 2c_i}{2} - s_i \Delta z^2\right)P_i + \frac{c_{i+1} + c_i}{2}P_{i+1} = -q_i \Delta z^2 \; . \; (5)$$

The error in the finite difference approximation is on the order of Δz^2 [5].

Now we need to define boundary conditions at each end of the pipe. We assume that the gas flow at each end is specified and that the conductance at the boundary is constant. In general, we have:

$$Q = -c\frac{dP}{dz} \quad \text{so}$$

$$Q_i = -c_i \frac{P_{i+1/2} - P_{i-1/2}}{\Delta z} \quad \text{or}$$

$$Q_i = -c_i \frac{P_{i+1} - P_{i-1}}{2\Delta z} \qquad (6)$$

This then allows us to solve for either P_{i+1} or P_{i-1} in eq. (5) in terms of the flow in the ith segment. So for the first segment we have (with $c_{i-1} = c_i = c_1$)

$$\left(-\frac{c_2 + 3c_1}{2} - s_1 \Delta z^2\right)P_1 + \frac{c_2 + 3c_1}{2}P_2 = -q_1 \Delta z^2 - 2Q_1 \Delta z \qquad (7)$$

and for the last segment we have (with $c_{i+1} = c_i = c_n$)

$$\frac{c_{n-1}+3c_n}{2}P_{n-1}+\left(-\frac{c_{n-1}+3c_n}{2}-s_n\Delta z^2\right)P_n=-q_n\Delta z^2-2Q_n\Delta z\,. \quad (8)$$

Now one can form a tridiagonal matrix from these equations.

$$\begin{pmatrix} -\frac{c_2+3c_1}{2}-s_1\Delta z^2 & \frac{c_2+3c_1}{2} & & & & \\ \cdot & \cdot & \cdot & & & \\ & \frac{c_i+c_{i-1}}{2} & -\frac{c_{i+1}+c_{i-1}+2c_i}{2}-s_i\Delta z^2 & \frac{c_{i+1}+c_i}{2} & & \\ & & \cdot & \cdot & \cdot & \\ & & & \frac{c_{n-1}+3c_n}{2} & -\frac{c_{n-1}+3c_n}{2}-s_n\Delta z^2 \end{pmatrix}\begin{pmatrix} P_1 \\ \cdot \\ P_i \\ \cdot \\ P_n \end{pmatrix}=\begin{pmatrix} -q_1\Delta z^2-2\,Q_1\Delta z \\ \cdot \\ -q_i\Delta z^2 \\ \cdot \\ -q_n\Delta z^2-2\,Q_n\Delta z \end{pmatrix}$$

This system of equations is easily solved using the techniques of *Gaussian elimination* and *back substitution* [6].

THE PROGRAM VACCALC.

A program called VACCALC has been made that utilizes the finite difference method mentioned above. The program accepts as input a file that lists the characteristics of each beam pipe element. The unit of length is the meter. The user specifies the segment length (Δz) on the second line of the input file. All the beam elements must have a length that is a multiple of the segment length. The program will round the length of beam pipe elements to the nearest multiple of the segment length. Any element that is shorter than the segment length is set equal to the segment length. A total of 10,000 segments are allowed for each pipe. This corresponds to a resolution of 1 mm for a 10 m long pipe or 1 cm for a 100 m long pipe [7]. An example of an input file is shown below. Figure 3, at the end of the paper, displays the output generated by VACCALC from this input file.

```
                1         2         3         4         5
Col.   12345678901234567890123456789012345678901234567890
Line
1      General label for input file.
2         0.001
3      Beam line label.
3         0.0       0.0         1    2        LIN  100
3       PIPE        2.0       50.0       20.0      100.0
4       PUMP        0.1       50.0       20.0     1000.0
5       PIPE        1.5       50.0       20.0      100.0
```

```
6      GAS          0.1      50.0     200.0       0.0
7      PIPE         1.5      50.0      20.0     100.0
8      PUMP         0.1      50.0      20.0    1000.0
9      PIPE         2.0      50.0      20.0     100.0
10     GAS    L     0.1     500.0      20.0       0.0
11     PIPE         2.0      50.0      20.0     100.0
12    ENDPIPE

                1         2         3         4         5
Col.   12345678901234567890123456789012345678901234567890
```

↑ Name four characters ↑ Distributed or lumped ↑ Length meters ↑ Conductance ↑ Outgas rate ↑ Pumping speed

The first line in the file is a title for the entire input file. The title can be up to 80 characters long.

The next line contains the segment length (Δz). The third line is a title for the following beam line. This title can also be up to 80 characters long. The fourth line contains the flow specifications at each end of the following beam line, the node identification number for each pipe end, the option of plotting the pressure profile with a linear or logarithmic scale, and a scaling factor that reduces the number of points to be used in the plots. A positive flow means that gas is coming into the first element of the line and going out of the last element of the line.

The units for incoming and outgoing flow are nTorr(l/s). The default is to plot the pressure using a linear scale. However, the scale can be changed to logarithmic by inserting "LOG" in columns 38-40. The scaling factor for the number of points in the plots is the number of pressure points to skip between plot points (i.e. a number of 10 would mean that every 10th calculated pressure point is plotted).

Following line four is a list of pipe elements. Each element can have a name with a maximum of 4 characters. The element can be either "lumped" or "distributed". A distributed element is the default. In this case, the units for conductance, outgas rate and pump speed are: m(l/s), nTorr(l/s)/m, and (l/s)/m respectively. An element that has an "L" in the 9th column is classified as a lumped element. In this case, the values of conductance, outgassing, and pump speed are assumed to be the total values for this element and the units are then l/s, nTorr(l/s), and l/s respectively. The program then divides the outgassing and pump speed values by the length of the element and multiplies the conductance by the length to get the specific or distributed values.

The end of a pipe is specified by a line with the word "ENDPIPE". The program then looks for the start of another pipe. If the ENDPIPE line is not used to finish off a file, the program assumes that the user had meant to put one in and continues on as though there had been one.

The node identification numbers are used to connect the ends of separate pipes together. If two pipe ends have the same node number then the program assumes that these two pipes are attached at the ends that have the same number. The gas flow at these ends is then considered a variable and the flow is adjusted through an iterative procedure until the pressure at the end of each attached pipe is the same. This method automatically insures that the sum of the flows at a given node is zero. Any number of pipe ends can be joined together at the same node. The program accepts a maximum of ten different pipes. The two ends of the same pipe can be given the same node number as well. When this is done, the program will set the pressure and flow at one end of the pipe equal to the pressure and flow at the other end. This periodic solution is useful for cases in which the design has a repetitive beam pipe construction (i.e. arc sections).

AN EXAMPLE.

We can compare results from the program described above with an analytic solution for a simple case. Figure 1 displays the geometry of a simple beam pipe. The pipe has conductance c_1 = 400 m(l/s) for 1 meter of length. Then the conductance changes to c_2 = 100 m(l/s) for the next meter of pipe. The final meter has a conductance that is equal to the first meter and also contains a distributed pump of 500 (l/s)/m. There is a gas flow of 100 l/s coming into the first section of the pipe. There is no outgassing from the pipe itself. Figure 2 shows a picture of the output from a Top Drawer file made by the program. The analytic solution is overlaid on this graph.

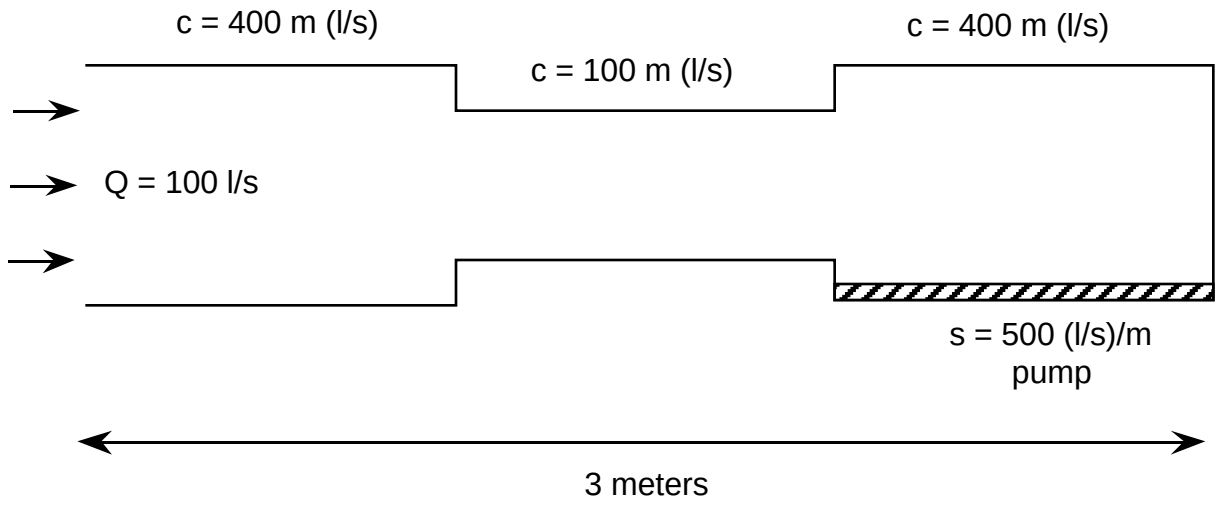

Figure 1. Schematic of the simple beam pipe structure mentioned in the text used to compare the finite difference procedure with an analytic solution.

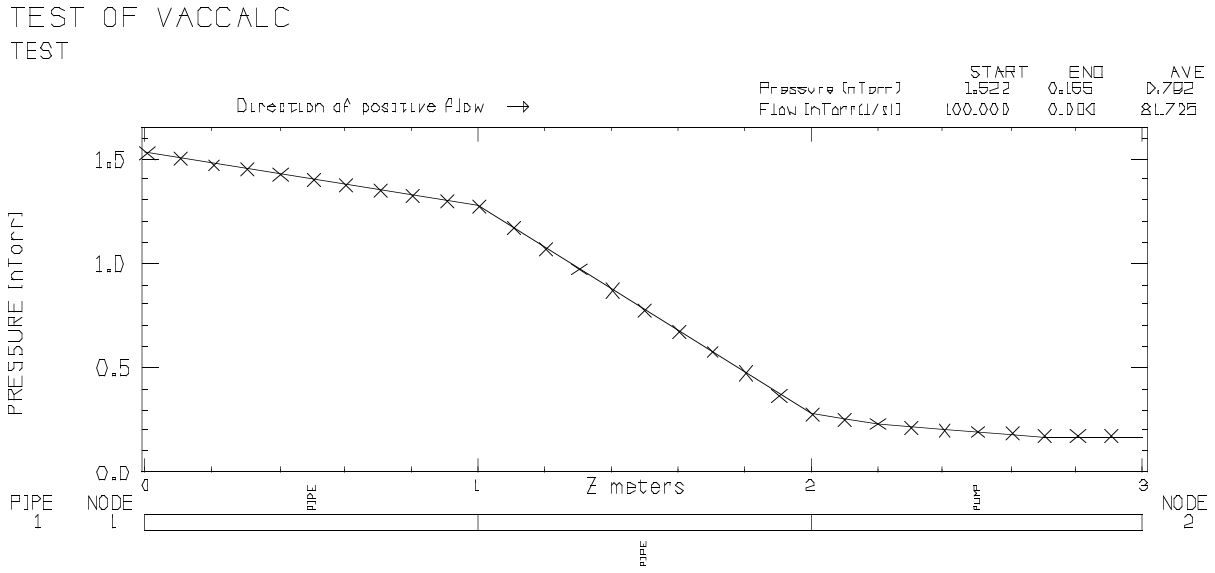

Figure 2. Plot of the pressure profile for the beam pipe in figure 1. The solid line is the analytic solution and the diagonal crosses indicate the values found by the finite difference method. The program calculated 300 pressure points and displayed 30 points.

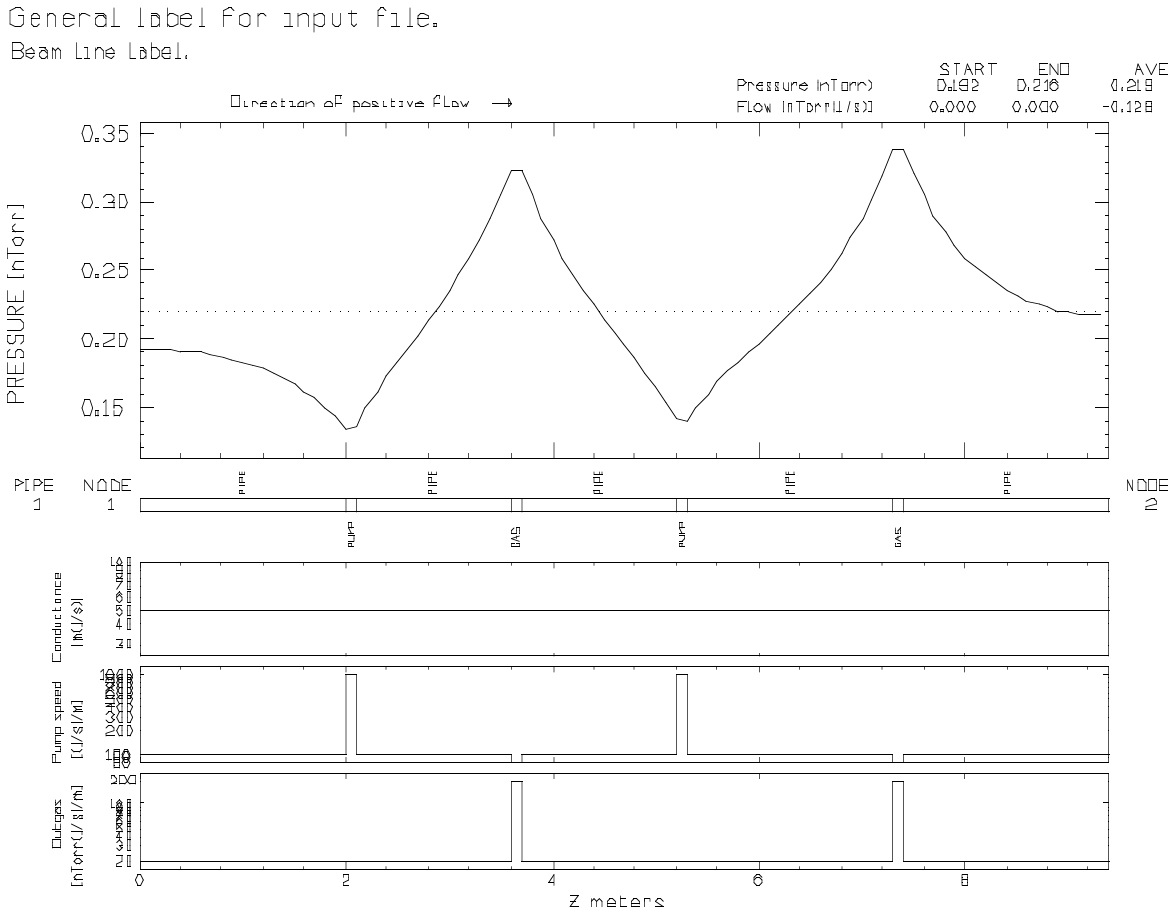

Figure 3. Output from VACCALC for the sample input file discussed in the text.

CONCLUSIONS.

The finite difference method is an effective mathematical procedure for calculating gas pressure profiles in beam pipes in which the gas is in the free molecular flow regime (viscosity is negligible). The procedure is numerically stable and pressure profiles from very long beam pipes can be readily calculated. A computer program is described that implements the finite difference method outlined in the text. The program is fast and, in addition, can calculate pressure profiles of complicated beam pipe structures such as those found in B factory designs where two independent storage rings merge into a common beam pipe at the collision point.

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REFERENCES.

[1] K. Kanazawa, *"On the pressure distribution of a ring accelerator: a Green's function approach"*, J. Vac. Sci. Technol **A6 (5)** (1988) pg. 3002.

[2] M. Michel, *"Calculation of pressure profiles in accelerators using a matrix method"*, Nucl. Inst. and Meth. **A322** (1992) pg. 1.

[3] With a few exceptions, I will follow the notation defined by Volker Ziemann in his note *Vacuum Tracking* SLAC-PUB-5962

[4] J. Ortega, W. Poole, *An Introduction to Numerical Methods for Differential Equations*, Pitman (1981). Chapter three has an excellent discussion on the derivation of the finite difference equations found for equation (3) in the text.

[5] *Ibid*. pg 75.

[6] B. Carnahan, H. Luther, J. Wilkes, *Applied Numerical Methods*, Wiley (1969) pgs. 269-270, 443-446.

[7] Numerical accuracy is controlled by the size of Δz with respect to the nominal numbers of the pipe. A 1 mm resolution for a 10 m pipe corresponds to a Δz of approximately one part in 10^4 for pipe element specific values of conductance, pumping and outgassing near one. Looking at eq. (8), we see that the accuracy of the finite difference values is set by Δz^2 or one part in 10^8. REAL*4 precision is only about 6-7 digits which is not quite good enough, especially if the conductance values of the pipe are much larger than one. The program therefore uses REAL*8 precision or about 15 digits of numerical accuracy. This is more than enough numerical precision for the maximum range of 10,000 pipe segments allowed by the program.